

Exhibit A

W0102

Rapid, Automated Molecular Replacement Using an Evolutionary Search Algorithm. Charles R. Kissinger, Daniel K. Gehlhaar and David B. Fogel*, Agouron Pharmaceuticals, Inc. 3565 General Atomics Court, San Diego, CA 92121 and *Natural Selection, Inc., 1591 Calle de Cinco, La Jolla, CA 92037

We have developed a new method for molecular replacement (MR) calculations that uses an evolutionary search algorithm to perform an efficient six-dimensional search. In this method, a population of initially random MR solutions is gradually optimized with respect to the correlation coefficient between observed and calculated structure factors. The method is several orders of magnitude faster than a systematic six-dimensional search. Comparisons with conventional MR techniques indicate that solutions can be found using significantly less accurate or less complete search models. A program incorporating this method, EPMR, has been developed which allows the rapid and highly automated solution of MR problems involving single and multiple molecules in the asymmetric unit. The program is now in use in a number of labs and has been used to solve several difficult MR problems. We are now investigating several ways of enhancing the method, including allowing the internal optimization of the search model geometry and selection between alternative search models during the evolutionary search.

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